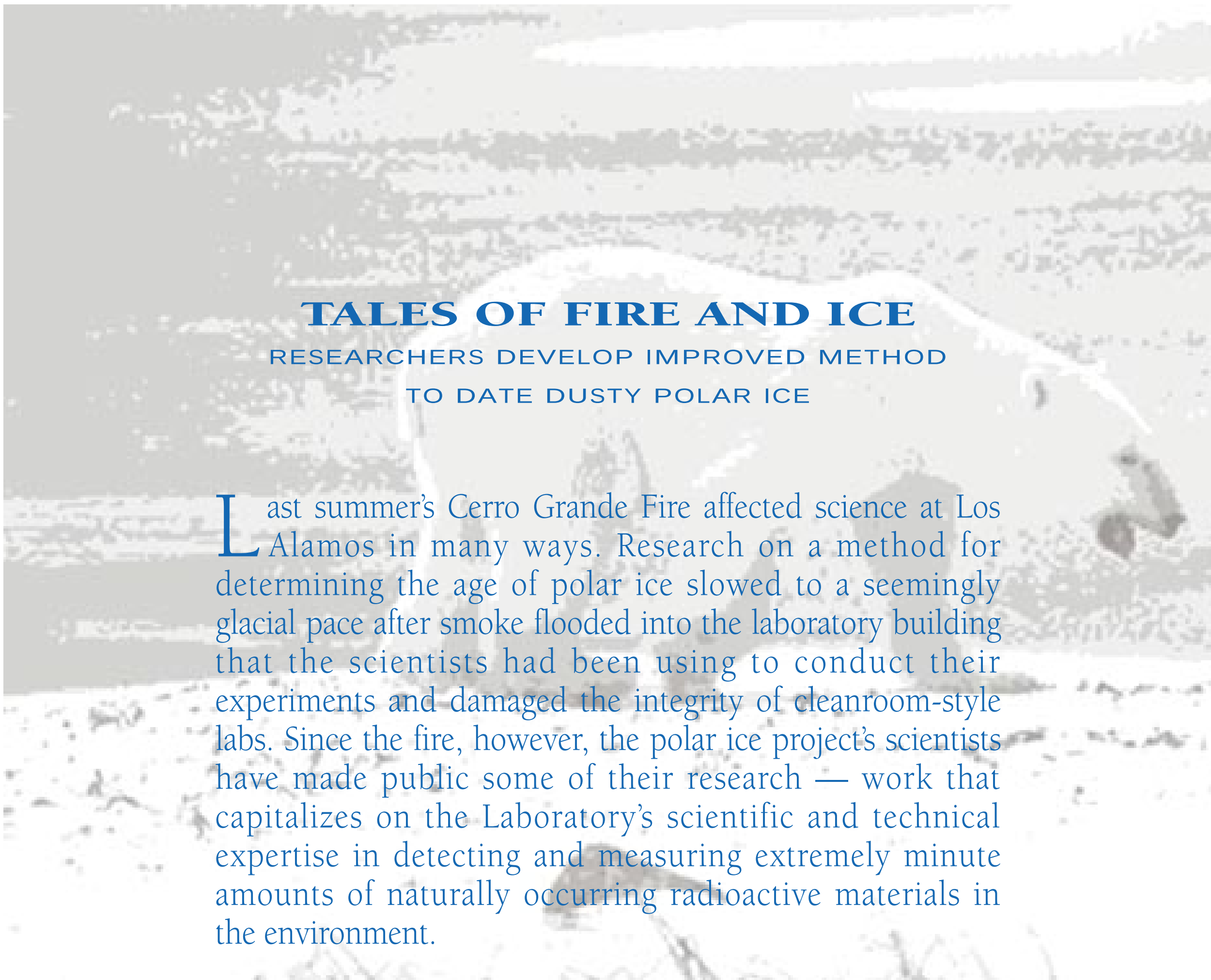
DECEMBER ISSUE 2000

LOS ALAMOS NATIONAL LABORATORY
WHERE SCIENCE MAKES A DIFFERENCE

DATELINE LOS ALAMOS

U.S. DEPARTMENT OF ENERGY
UNIVERSITY OF CALIFORNIA



TALES OF FIRE AND ICE

RESEARCHERS DEVELOP IMPROVED METHOD TO DATE DUSTY POLAR ICE

Last summer's Cerro Grande Fire affected science at Los Alamos in many ways. Research on a method for determining the age of polar ice slowed to a seemingly glacial pace after smoke flooded into the laboratory building that the scientists had been using to conduct their experiments and damaged the integrity of cleanroom-style labs. Since the fire, however, the polar ice project's scientists have made public some of their research — work that capitalizes on the Laboratory's scientific and technical expertise in detecting and measuring extremely minute amounts of naturally occurring radioactive materials in the environment.

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Steven Goldstein, Michael Murrell and Andrew Nunn of Los Alamos' Chemistry Division recently revealed a direct radiometric dating method that could allow scientists to refine existing age estimates of polar and glacial ice. These researchers used dusty ice samples taken from the ice fields near Allan Hills, a 12-mile-long group of hills located along the coast of the Ross Sea in Antarctica known for its abundance of meteorites, to test this dating technique. In the process, the researchers not only demonstrated an improved methodology for dating ice but unintentionally challenged some existing dogma in the field of glaciology along the way.

Currently, scientists interested in determining the age of ice sheets may either count the visible bands or layers in the ice or employ traditional carbon-14 dating methods. While both methods are widely applied, each has limitations.

Band counting can't really account for any missing sections in the ice column, and carbon-14 is generally useful for dating back only about 40,000 years.The Los Alamos method, because it could be applied more widely than counting banding, and since it works on a time scale well beyond that of carbon-14 dating, might soon be used to address several unsettled issues in the study of ancient climates and glaciers.

In paleoclimatology, a more precise method for dating ice older than 20,000 years could help resolve the existing controversy over

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the chronology of the last interglacial period shown in Greenland ice cores. Contrary to other evidence, the Greenland ice cores show large and rapid climate fluctuations that may very well be analogous to our current climate.

A new method may also help answer a key question in current paleoclimate research regarding the disparity between the continental and marine records. Marine coral records of sea-level fluctuation indicate the onset of the last interglacial period to have been 122,000 to 130,000 years ago. Conflicting studies of the Great Basin calcite vein record, where ground water flowing out though an open fault zone near Ash Meadows, Nev., provides a calcite rock record of continental climate, puts the period at closer to 140,000 years ago.

In glaciology, improved dating methods could be used to better understand the physical movement of ice sheets and perhaps the terrestrial history of Antarctic meteorites.

The radiometric dating method developed at Los Alamos uses mass spectrometry to make extremely sensitive measurements of minute amounts of uranium-series elements that are naturally present in polar ice. The uranium-series elements are uranium, radium, thorium and protactinium.

←

Kunihiko Nishiizumi uses a chain saw to collect an ice sample from directly under the meteorite Allan Hills 82102 as Paul Pellas, formerly of the Laboratoire de Mineralogie du Museum in Paris, France, looks on. The ice in which the meteorite was embedded was part of the Allan Hills Far Western Icefield,Victoria Land, Antarctica. At the time of the sampling, Jan. 2, 1984, Nishiizumi was with the University of California - San Diego and is now with the Space Sciences Laboratory at the University of California - Berkeley. The Antarctic research was funded by National Science Foundation. Studies of the meteorite and ice were published in Nature.

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Researchers determine the age of the ice by comparing infinitely small concentrations of uranium-series daughter isotopes, the natural products created by the radioactive decay of the elements, to their parent isotopes in the sample. The dating process itself can be complex and exacting because the quantities of natural radioactive elements the researchers measure are so small that they are in the femtogram, or one quadrillionth of a gram, scale.

A small portion of the Greenland ice core sample in the early stages of preparation for uranium-series radiometric dating.

Using samples gathered from Allan Hills to test the method, the team's uranium-series dating of the samples unexpectedly drew results that suggest a far younger age for the Antarctic ice than previously thought. Although earlier published data, based primarily on measurements made using alpha spectrometry, placed the age of the Allan Hills ice at roughly 325,000 years, Los Alamos data suggest that the age is only approximately 30,000 years. These results surprised the researchers and their colleagues.

Further work at Los Alamos to verify this result had been interrupted by the Cerro Grande fire. These test included uranium-series analyses of the dust bands present in Allan Hills ice, as well as dating studies of ice cores from the Summit region of central Greenland. Further tests aside, the Allan Hills results seem to offer promising uses for the new method, including applications in the field of meteorite studies.

Named for R.S. Allan of the University of Canterbury in New Zealand, the Allan Hills region is famous for its abundance of old meteorites, including 1 84001 — the controversial meteorite that produced much speculation about possible life on Mars.

By applying the uranium-series dating method to ice samples located near the sites where these fiery meteors came to rest on Earth, the terrestrial age of the meteorite and the ice age can be compared, yielding a better understanding of the terrestrial history of meteorites and ice sheets. Here, at this unlikely confluence of fire and ice, may lie a better understanding of our changing planet.

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AN ODD COMBINATION

CAN FISH BONES, PECAN SHELLS AND ROCKS CLEAN GROUNDWATER?

It may be the oddest combination of environmental remediation tools ever assembled: fish bones, pecan shells, volcanic rock and limestone. But laboratory-scale tests at Los Alamos show that this “quaint quartet” may greatly reduce — possibly even eliminate — radionuclides, nitrates, perchlorate, high-explosive residues and heavy metals from groundwater.

Los Alamos is preparing to field test this conglomeration sometime next summer in a canyon where liquid waste containing low levels of nitrates, perchlorate and radionuclides is being discharged. If successful, research institutions and industry nationwide may have an inexpensive tool for cleaning contaminated groundwater.

The bones, shells and rocks are configured into layers and placed side-by-side to form a multibarrier. The first layer is a colloid barrier consisting of volcanic rock treated with a commercially available cationic polymer (called Catfloc) that serves as a particle flocculent, which attracts particles together to form a suspension (or mass). The polymer has a positive charge that attracts the negatively charged colloids — tiny particles that can attach onto and transport radionuclides — and traps them.

The second layer consists of the fish bones. All bones contain apatite, a calcium mineral that traps radionuclides such as strontium, plutonium and americium, and removes them from the groundwater.

The pecan shells make up the third layer, which supports the growth of microbial species that destroy nitrates and perchlorate. The last layer is a polished limestone that absorbs whatever radionuclides

Fish bones, pecan shells, volcanic rock and limestone are being combined to form a barrier to clean groundwater.

manage to pass through the first three layers and restores the pH level of the groundwater that is lowered slightly as it passes through the initial parts of the multibarrier.

In lab-scale tests, researchers spiked water with the radionuclides americium (83 nanocuries), plutonium (741 nanocuries) and strontium (14 microcuries). They used groundwater with nitrates at about 30 parts per million and perchlorate at 350 parts per billion, then ran the water through the multi-barrier over a two-week period, simulating the rate of groundwater movement.

Initial results showed that the radionuclides were removed to below-detection levels. Nitrates were destroyed, and the level of perchlorate remaining in the water was below the proposed Environmental Protection Agency standard of 18 parts per billion. In separate tests, the multibarrier was shown to remove up to 600 parts per million of nitrates effectively.

While the multibarrier has not yet been tested on high-explosive residues and heavy metals, Los Alamos researchers say data suggest it could work on them as well. Researchers also say the multibarrier can continuously remove all of these contaminants for about 10 years, possibly longer.

Perchlorate is a chemical compound used in a variety of industrial processes. It has been identified by the EPA as a contaminant of concern. Nitrates are essentially nitric acid salts and are wastes typically generated in the mining, chemical, farming and nuclear industries. Nitrates can cause excessive biological activity and vegetation growth and result in precipitation of organic residues from microbial metabolic processes when brought into contact with bodies of water. If consumed in sufficient quantities, nitrates can harm humans, especially infants.

Radionuclides are specific atoms that emit radioactivity and are denoted by their atomic mass and weight, such as strontium-90, which is produced in nuclear explosions and is the principal health hazard in radioactive fallout. High-explosive charges can leave metal residues in the soil and contaminate groundwater.

Current plans call for placing the multibarrier as far west as can be accessed in a Laboratory adjacent canyon, where researchers need only dig about 15 feet to reach the groundwater. Researchers approximate that the multibarrier will be 20-to-30-feet long and cover the width of that section of the canyon (about 70 feet) to ensure that no groundwater escapes. Special monitors called lysimeters will be placed along the 30-foot path to monitor the barrier's effectiveness.

Los Alamos' Chemistry Division is assisting the Environmental Technologies Group to conduct the lab tests, and the Earth and Environmental Sciences Division and Environment, Safety and Health Division are helping support the field test and analyses.

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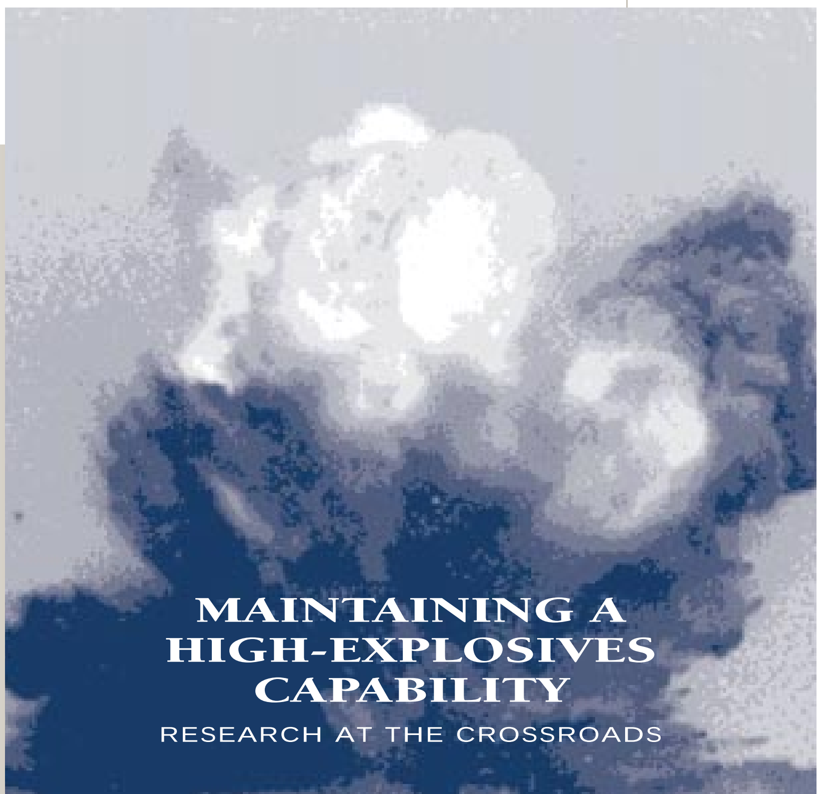

Research into energetic materials at Los Alamos is at something of a crossroads. Do we continue to build on work rooted largely in the past, or forge ahead, breaking new ground?

"The simple fact is that an energetic materials synthesis capability is on a decline in this country," said Los Alamos researcher Michael Hiskey. "There's just not a major need for new high-performance energetic materials out there in the general market."

But in the area of national security it is vitally important to maintain the capability. Issues such as the safety and reliability of aging systems and their refurbishment or replacement, terrorist and proliferant threats, and the unknown challenges of the future underscore the need for a national program at the forefront of new developments and technologies. The Departments of Defense and Energy both recognize this and have turned to Los Alamos as one of the last places in the United States with the people and the facilities that can get the job done.

Research in energetic materials at Los Alamos dates back to the Manhattan Project. Research worldwide goes back almost another hundred years, when, as an alternative to gunpowder, Alfred Nobel and his father began exploring the properties of nitroglycerine, an unstable but highly energetic compound discovered by Italian chemist Ascanio Sobrero in 1847.

It wasn't until 1866, following a series of spectacular and deadly accidents at his factories, that Nobel had the idea of mixing nitroglycerine with the absorbent clay kieselguhr, and thereby inventing the much more stable explosive we now know as dynamite, the first real high explosive.

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The ideas that led to dynamite have continued to evolve. In the 1940s new classes of high explosives were employed in the Manhattan Project. The familiar trinitrotoluene (TNT) and less familiar British-invented Research Department Explosive (RDX) were combined to create "Composition B" and, along with Baratol, were used in the first implosion atomic bombs, the Trinity Device and Fat Man, the bomb dropped on Nagasaki.

At the Manhattan Project lab, explosive "lenses" — specially shaped high explosives with a slow burning core surrounded by a fast burning exterior — were fabricated by casting liquid slurry into molds, hardening them and precisely machining the molds into specific shapes. The lenses were positioned so that when detonated around a core of fissile material, they produced a uniform shock wave that induced a nearly perfect spherical implosion. That implosion compressed a plutonium core into a critical mass and thus, the incredible power of the atomic bomb.

One goal of high-explosives, or HE, science at Los Alamos is to maintain a world-class base of knowledge for better understanding and responding to changes in the Lab's weapons capability. This could be accomplished without pushing the outside of the envelope, but that's not the way things are done at Los Alamos, if you ask the people who have the "Right Stuff" in the Dynamic Experimentation Division.

"We had to ask ourselves, if we're going to maintain this capability, should we just rest on the laurels of the past or should we go out on a limb a little?" said Hiskey. "We've decided to forge ahead with work on a new classes of energetic materials."

This high-nitrogen-content material burns with an extremely bright flame. Because of their combustion properties, high-nitrogen compounds yield less carbon than other materials that rely on combustion from a carbon backbone.

RESEARCH TODAY

Research efforts at Los Alamos continue to focus on the HE triad of performance, safety and reliability. "We have a very diverse and active HE program at the Lab," said researcher Alan Picklesimer. "And the work we are doing is not being done anywhere else."

The wide spectrum of HE research at the Lab includes exploring the performance-based issue of equation of state, or that equation that dictates a certain material's properties based on volume, pressure and thermodynamics. For HE, that means a

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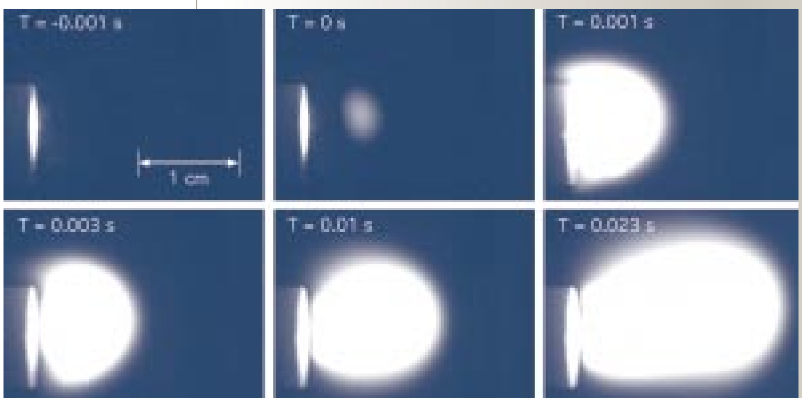


HERCULES, or High Explosive Reaction Chemistry by Ultrafast Laser Excited Spectroscopies, uses extremely short laser bursts, quadrillionths of seconds in length, to get a clear picture of the shock front in a detonation wave.

numerical description of how the product gases drive metal.

HERCULES, or High Explosive Reaction Chemistry by Ultrafast Laser Excited Spectroscopies, uses extremely short laser bursts, quadrillionths of seconds in length, to get a clear picture of the shock front in a detonation wave. Fast-scale chemistry is explored to determine the chemical kinetics in a burn-front to understand better the chemical reactions, how the system develops and which reactions work the fastest with the greatest efficiency, with the ultimate goal of understanding the material's ability to drive things.

The basic physical properties of HE — such as the strength of the material and how it reacts and responds to thermal and mechanical insults — also are studied in depth. HE materials are cooked and frozen, dropped and crushed, shot with bullets and set on fire, all to better know why and how the materials work, and to constantly improve both their performance and safety.

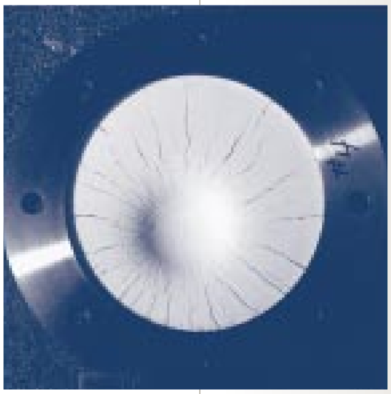
Hiskey's focus is on high-nitrogen energetic materials, or HiN, in the pursuit of discovering compounds with superior performance without sacrificing stability.

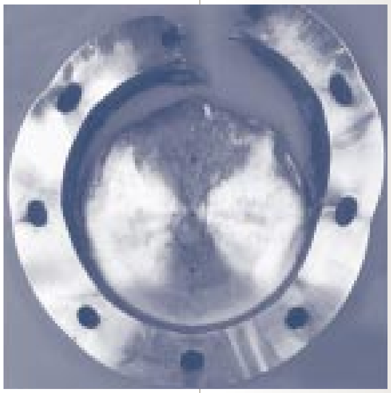
This performance vs. sensitivity equation drives the Los Alamos effort to make practical and useful materials. Such materials are key to updating the aging nuclear weapons stockpile with HE components that are safe, long-lasting, reliable and more environmentally friendly.

HOW HIGH EXPLOSIVES WORK

Explosives, in general, employ fairly simple combustion reactions, in which fuel and an oxidizer are mixed at the molecular level. The four elemental components of explosives are carbon, hydrogen, nitrogen and oxygen, and it's the ratio of these elements that govern the properties of the final product. HiN materials derive most of their energy from very high "heat of formation" — energy liberated or absorbed by a certain amount of a compound as it is formed from its constituent elements.

"The synthesis of compounds known as high-nitrogen energetic materials have been the focus of our group for the past decade," said Hiskey. "These compounds form a unique class of energetic materials deriving most of their energy from their very high positive heats of formation, rather than from oxidation of the carbon backbone, as with traditional energetic materials."





A sample of the high-explosive PBX 9501 shows deformation after being impacted at 65.5 meters per second. A second sample reacted violently and broke the sample holder when impacted at 80.7 meters per second.

The high nitrogen content typically leads to high densities, and the low amount of hydrogen and carbon also allows for a good oxygen balance, a measure of the oxygen to fuel ratio in a compound, to be achieved more easily. HiN materials have been demonstrated to be remarkably insensitive to electrostatic discharge, friction and impact.

Los Alamos is one of the few research institutions in the world with a continuing capability in HE synthesis research and looks forward to future work with HiN compounds in the quest for stable, reliable and environmentally benign energetic materials.

Other work that is unique to Los Alamos includes a project that imbeds small magnetic sensors inside the HE and then shocks the material to study the wave propagation inside the HE itself.

"This work is wonderful for the theorists and modelers," said Picklesimer. "It results in a picture of what is happening within the HE during a detonation sequence, and again, there's no one else doing this type of work."

INTO THE FUTURE

In terms of extreme future-think, there is work with Metastable Intermolecular Composites (MICs) that seeks to exploit nanoscale technology to create exothermic, or heat producing, reactions in metals like aluminum and molybdenum. These types of 21st century, next-generation gunpowders could prove valuable as completely new forms of HE or rocket propellants.

Research and development of energetic materials continues at Los Alamos both for maintaining a capability and breaking new ground. "We do it because it's in the national interest to keep abreast of the newest developments in HE science," said Picklesimer. "We simply cannot, and will not, be left behind in this important area of science."

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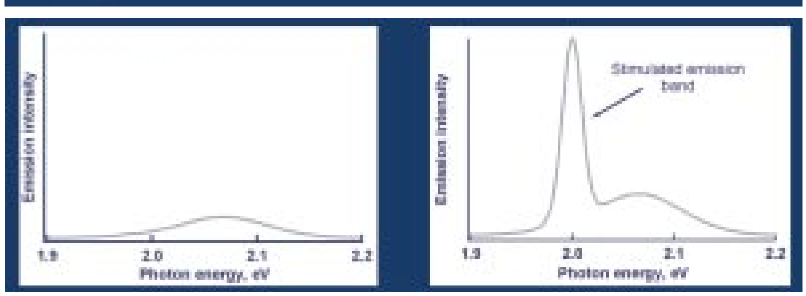
NANOCRYSTAL QUANTUM DOTS

RESEARCH MAY LEAD TO DEVELOPMENT OF NOVEL LASERS AND AMPLIFIERS

Scientists at Los Alamos and the Massachusetts Institute of Technology have demonstrated that nanoscale semiconductor particles called "nanocrystal quantum dots" offer the necessary performance for efficient emission of laser light. The research opens the door for developing novel optical and optoelectronic devices, such as tunable lasers, optical amplifiers and light-emitting diodes, from assemblies of these invisibly small particles.

"Our results provide a proof-of-principle and should motivate the development of nanocrystal quantum-dot-based lasers and amplifiers," said Los Alamos' Victor Klimov. The research appeared in the Oct. 13 issue of *Science*.

Quantum dots are so small that quantum mechanical effects come into play in controlling their behavior. Quantum mechanics applies in the microscopic realm but its effects are largely unseen and unfelt in our macroscopic world.



The image at left shows the development of an intense narrow-band simulated emission in solid-state film. The spectra below show the emitting sample before and after the lasing threshold.

Quantum dot lasers work like other semiconductor lasers, such as those found in home-audio compact-disc players. Just as in the semiconductor laser chip in a CD player, the goal of a quantum dot laser is to manipulate the material into a high-energy state and then properly convert it to a low-energy state. The result is the net release of energy, which emerges as a photon.

The challenge, however, is that there are competing mechanisms by which the energy can be released, such as vibrational energy or electron kinetic energy. In quantum dots, the electrons are confined within a very small volume that forces them to strongly interact with each other. These strong interactions can lead to deactivation of the dot through the so-called "Auger process," preventing it from emitting a photon.

The Los Alamos-led researchers examined quantum dots formed of several types of crystalline material. They showed that the quantum dots exhibit sufficiently large optical gain for stimulated emission to overcome the nonradiative Auger process. Stimulated emission, or lasing, was only possible, however, when the dots were densely packed in the sample.

Quantum dots offer this performance over a range of temperatures, making them suitable for a variety of applications, and they also can be "tuned" to emit at different wavelengths, or colors. The emission wavelength of a quantum dot is a function of its size, so by making dots of different sizes scientists can create light of different colors.

The quantum dot material is easily manipulated through well-established chemical synthesis methods. Fabricating densely packed quantum dot arrays should be a straightforward material processing challenge.

The Los Alamos team conducted most of its research before this summer's Cerro Grande Fire, which hit the group very hard. Several postdoctoral researchers on the team lost data and equipment in the fire and much of Klimov's optics equipment was damaged. (See *Dateline: Los Alamos* Summer 2000.)

In Los Alamos, the quantum dot research was funded by the Laboratory Directed Research and Development Program.

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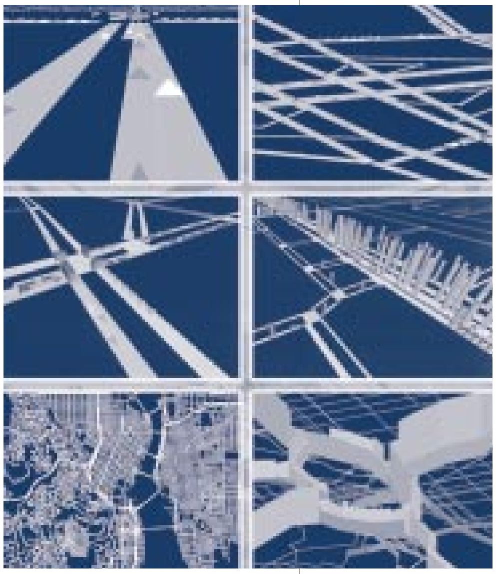
DATELINE FOLLOWUP

TRANSIMS GETS CORPORATE PARTNER

Los Alamos is teaming with PricewaterhouseCoopers to take TRANSIMS, a remarkable traffic simulation software package developed at the Lab, and create products that can be deployed to metropolitan planning agencies nationwide.

Funded by the U.S. Department of Transportation over the last six years at a cost of $25 million, the TRANSIMS simulation software represents a major advance in transportation-flow forecasting procedures.



TRANSIMS provides planners with a synthetic population's daily travel patterns, simulates the movements of individual vehicles on a regional transportation network and estimates the air pollution emissions generated by vehicle movements. (See *Dateline: Los Alamos* April 1998.)

TRANSIMS makes use of advanced computer simulation codes developed originally for national security purposes and run on computers at Los Alamos' Advanced Computing Laboratory. PricewaterhouseCoopers will further develop the user interface software and package the TRANSIMS software to create a version useable for state and local planning agencies.

Spin-off applications of the simulation software have already been used by Los Alamos scientists to model the movement of travelers through airborne toxins such as might be released in a terrorist attack. Now Los Alamos is exploring EpiSim, an application of TRANSIMS that integrates disease models with patterns of interpersonal human contact. EpiSim will allow health-care organizations to make more accurate predictions of the spread of epidemics in this era of high mobility.

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SCIENCE FOR THE 21ST CENTURY

HYDROMODELING

EXPLORING GLOBAL WATER ISSUES

Hydromodeling will include advances in the use of supercomputers to create hydrological models that simulate oceans, rivers and streams and allow researchers to explore crucial national and global water management issues.

Earth's climate is controlled by a complex interaction of many physical systems, including the atmosphere, oceans, sea ice, land surface and the biosphere. The oceans are of key importance in understanding climate, because changes in ocean circulation patterns are important in determining climate variability on time scales of decades to centuries.

Deep ocean currents, for example, create a type of global conveyor belt that transports huge amounts of heat around the world. These ocean currents have the potential to affect significant climate change because of the intimate relationship between the ocean and the atmosphere.

Using Los Alamos' Parallel Ocean Program, scientists have completed a one-tenth-degree — the measure refers to angular spacing between grid points along the equator — computer simulation of the North Atlantic Ocean using available wind surface data from 1985 to 1995. Computer simulations help scientists learn how oceans interact and develop a better understanding of global-scale circulation patterns.

Because Los Alamos is located in the semiarid southwestern United States, scientists also are aware of the importance of water management. They have used Los Alamos supercomputers to create a model of water resources in the Rio Grande Basin and recently completed their first soil-moisture maps of the Upper Rio Grande Basin. Research so far has focused mainly on land-surface and atmospheric interactions.

Los Alamos is part of a consortium led by the National Science Foundation and the University of Arizona collaborating on a five-year, $16 million project to develop a virtual watershed laboratory in which scientists can conduct experiments on simulated watersheds that faithfully reflect the physics of real watersheds.

The collaboration will allow scientists to test hypotheses by manipulating variables such as population and analyzing the effects of these changes on dependent variables such as soil moisture and water flow.

Scientists also can attempt to answer questions about how watersheds are affected by climate changes, population growth and changes in water allocation systems that de-emphasize agriculture. The research will help water management experts advise policy makers who will set water use priorities for present and future generations.

By providing researchers a computing environment in which to conduct these simulations, the National Science Foundation Science and Technology Center, in conjunction with Los Alamos scientists, also hope to make the general public more "hydrologically literate" and expand people's understanding of the water supply.

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BRIEFLY . . .

THOMAS TERWILLIGER OF LOS ALAMOS' BIOSCIENCES DIVISION HAS BEEN ELECTED A FELLOW OF THE AMERICAN ASSOCIATION FOR THE ADVANCEMENT OF SCIENCE. Terwilliger was elected a Fellow by the AAAS Council "for fundamental advances in macromolecular crystallography and protein chemistry, including development of the first software capable of automated macromolecular X-ray structure solution."

Along with his colleague Joel Berendzen of the Physics Division, Terwilliger developed computer software called SOLVE that has made it possible to "see" the shapes of protein molecules more easily. SOLVE is an expert system that automatically produces three-dimensional pictures of protein molecules from X-ray diffraction measurements. Pictures of protein molecules are in high demand in biotechnology for drug discovery and for engineering enzymes for commercial use.

AAAS is a nonprofit professional society dedicated to the advancement of scientific and technological excellence across all disciplines and to the public's understanding of science and technology. Terwilliger will be honored in February in San Francisco during AAAS' Fellows Forum, part of the organization's annual meeting. AAAS membership comprises more than 143,000 scientists, engineers, science educators, policymakers and other professionals worldwide. As a Fellow, Terwilliger joins an elite group of about 10,000 of the nation's leading researchers.

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